

Triisopropanolamine
122-20-3 | DTXSID5021415

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 38.8 °C

Global applicability domain: Inside

Local applicability domain index: 4.39e-01

Confidence level: 5.69e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Triisopropanolamine</div> <div>Measured: 45.0</div> <div>Predicted: 38.8</div>	<div>Image not found</div> <div>Triethanolamine</div> <div>Measured: 20.5</div> <div>Predicted: 24.5</div>	<div>Image not found</div> <div>Diisopropanolamine</div> <div>Measured: 44.5</div> <div>Predicted: 46.5</div>
<div>Image not found</div> <div>2,2'-(tert-Butylimino)diethanol</div> <div>Measured: 42.0</div> <div>Predicted: 24.4</div>	<div>Image not found</div> <div>Ethyl diethanolamine</div> <div>Measured: -50.0</div> <div>Predicted: -29.9</div>	